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An Euler-Bernoulli second-strain gradient beam theory for cantilever sensors

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1 Introduction

Because of their high surface over volume ratio, the mechanical behavior of micrometer sized structures differs from that of usual macroscopic objects. Their surface plays a key role, and this property has been proposed to devise micromechanical sensors of environmental changes [1]. In particular, a significant effort has been put on the development of biological sensors [2], thus highlighting the need for a more basic understanding of coupled surface phenomena [3].

These micromechanical sensors are usually operated in either static or dynamic mode. The latter allows one to detect the change in mass experienced by a micromechanical resonator. One

will focus herein on cantilevers operated in static mode : a micro-cantilever which is typically few hundreds of micrometer long and one micrometer thick is chemically functionalized on one side to react with a specific target molecule. It has been experimentally reported that when the chemical recognition mechanism occurs (on the modified side), it induces some micro-cantilever bending which may be detected through different ways. The available experimental material has been mostly obtained using the optical lever technique [4] which provides the (quasi-static) deflection at the cantilever tip. Such an arrangement allowed many groups to demonstrate such a chemo-mechanical coupling for a large variety of molecular interactions (see [5] for biological applications for instance). The quantitative (and sometimes qualitative) interpretation of the retrieved experimental data is however challenging. Several reasons make the investigations of these chemically-induced mechanical effects particularly difficult :

- These results are usually interpreted through Stoney's equation [6], which was developed to describe the mechanical state of thin metallic films deposited onto free substrates. This formulation makes use of many assumptions, the validity of which is questionable when dealing with chemically-induced effects.

- More elaborated frameworks are available in the literature. The concept of surface stress as presented in [7] for solids does not elucidate the connection between surface and bulk (Cauchy) stresses. This is however a key point for describing the translation from surface (chemical) to bulk (mechanical) effects. Gurtin and Murdoch [8] introduced a rigorous formulation for the mechanics of surfaces, making use of surface elasticity moduli. These can however be negative, and the meaning of such a situation is not clear. Asymptotic analysis is a thermodynamically grounded alternative approach [9], but which does not yield closed-form solutions for the displacement of chemically-modified cantilevers.
- In addition to this conceptual difficulty, one should add that some systems (such as DNA-DNA hybridization) yields somehow controversial experimental results [4] : for similar chemical conditions and mechanisms, the bending may be seen to occur towards or away the functionalized surface.

Starting from a insufficiently known contribution by Mindlin [10], a linear theory of deformation of elastic beams in which the strain-energy density is a function of strain and its first and second gradients is adopted. As Mindlin demonstrated that such a

theory is able to describe the surface tension for solids, this paper is intended to derive a tractable beam theory based on such a higher order material description. This contribution may therefore be seen as an extension of the recent propositions to describe the behavior of tiny Euler-Bernoulli [11–13] or Timoshenko [14] beams. The basic assumptions regarding the beam behavior are first presented. The virtual work principle [15] is then applied to yield the differential equations governing the mechanical behavior of chemically-modified isotropic beams. These equations are solved for cases of interest and the results are discussed.

2 Basic assumptions

Considering a beam lying along \mathbf{x} direction and using the Euler-Bernoulli assumption, the displacement \mathbf{d} for a loading in the (\mathbf{x}, \mathbf{y}) plane reads

$$d_x = u(x) - y \frac{dv(x)}{dx} \quad ; \quad d_y = v(x)$$

Following Mindlin [10], the free energy density is assumed to depend on the classical infinitesimal strain ϵ^1 , as well as on the triadic $\epsilon^2 = \nabla \nabla \mathbf{d}$ (symmetric in the first two positions) and on $\epsilon^3 = \nabla \nabla \nabla \mathbf{d}$ (symmetric in the first three positions). ϵ^1 has

therefore a single non-vanishing component

$$\epsilon_{xx} = -y \frac{d^2 v}{dx^2} + \frac{du}{dx}$$

The non-zero components of ϵ^2 read

$$\epsilon_{xxx} = -y \frac{d^3 v}{dx^3} + \frac{d^2 u}{dx^2} \quad ; \quad \epsilon_{xxy} = \frac{d^2 v}{dx^2} = -\epsilon_{xyx} = -\epsilon_{yxx}$$

The components of ϵ^3 read

$$\epsilon_{xxxx} = -y \frac{d^4 v}{dx^4} + \frac{d^3 u}{dx^3} \quad ; \quad \epsilon_{xxxy} = \frac{d^3 v}{dx^3} = -\epsilon_{yxxx} = -\epsilon_{xyxx} = -\epsilon_{xxyx}$$

The elastic behavior is assumed to be isotropic and is modeled according to the constitutive law derived by Mindlin [10]. The elastic behavior is thus described by five coefficients a_n (found in Toupin's theory describing surface effects for non-centrosymmetric materials [16]), a cohesion modulus b_0 , seven coefficients b_n and three coefficients c_n in addition to the Lamé coefficients λ and μ . The ratios a_n/μ , b_0/μ and c_n/μ scale as a squared length, and b_n/μ as a length to the fourth power.

3 Virtual work principle for a beam featuring a through-thickness modulus of cohesion gradient

Mindlin demonstrated that the cohesion modulus b_0 contributes to the free energy density through a term $b_0 \epsilon_{iijj}$ which is then linear with respect to the kinematic variables. It thus defines a surface energy (without any external loading), so that one will assume in the following that all the material parameters are homogeneous in the cantilever beam, except the cohesion modulus b_0 which is considered to possibly depend on y in order to describe the chemical modification of one cantilever side compared to the other. Considering a virtual displacement field \mathbf{d}^* , the virtual change in the potential energy density $W(\mathbf{d}^*)$ [15] reads

$$W(\mathbf{d}^*) = \tau_{xx} \epsilon_{xx}^* + \tau_{xxx} \epsilon_{xxx}^* + 2\tau_{yxx} \epsilon_{yxx}^* + \tau_{xxy} \epsilon_{xxy}^* + \tau_{xxxx} \epsilon_{xxxx}^* + 3\tau_{yxxx} \epsilon_{yxxx}^* + \tau_{xxyy} \epsilon_{xxyy}^*$$

with

$$\begin{aligned} \tau_{xx} &= (\lambda + 2\mu) \epsilon_{xx} + (c_1 + c_2 + c_3) \epsilon_{xxxx} \\ \tau_{xxx} &= 2(a_1 + a_2 + a_3 + a_4 + a_5) \epsilon_{xxx} \\ \tau_{yxx} &= (a_1 + 2a_4 + a_5) \epsilon_{yxx} + \left(\frac{a_2}{2} + a_5\right) \epsilon_{xxy} \\ \tau_{xxy} &= (a_2 + 2a_5) \epsilon_{yxx} + 2(a_3 + a_4) \epsilon_{xxy} \\ \tau_{xxxx} &= 2(b_1 + b_2 + b_3 + b_4 + b_5 + b_6 + b_7) \epsilon_{xxxx} \\ &\quad + \frac{b_3}{2} (\epsilon_{xxyx} + \epsilon_{xxxy}) + (c_1 + c_2 + c_3) \epsilon_{xx} + b_0(y) \end{aligned}$$

$$\begin{aligned}\tau_{yxxx} &= \frac{2}{3} (2b_2 + b_3 + b_5 + 3b_6 + 2b_7) \epsilon_{yxxx} + \frac{1}{3} (b_3 + 2b_4 + 2b_7) \epsilon_{xxxy} \\ \tau_{xxxy} &= (b_3 + 2b_4 + 2b_7) \epsilon_{yxxx} + 2(b_5 + b_6) \epsilon_{xxxy}\end{aligned}$$

Making use of the following substitutions

$$A = a_1 + a_2 + a_3 + a_4 + a_5 = (\lambda + 2\mu) l_A^2 \geq 0 \quad (1)$$

$$B = b_1 + b_2 + b_3 + b_4 + b_5 + b_6 + b_7 = (\lambda + 2\mu) l_B^4 \geq 0 \quad (2)$$

$$C = c_1 + c_2 + c_3 = (\lambda + 2\mu) l_C^2 \geq 0 \quad (3)$$

$$\tilde{A} = a_1 - a_2 + a_3 + 3a_4 - a_5 = (\lambda + 2\mu) l_{\tilde{A}}^2 \quad (4)$$

$$\tilde{B} = b_2 - b_4 + b_5 + 2b_6 = (\lambda + 2\mu) l_{\tilde{B}}^4 \quad (5)$$

and integrating $W(\mathbf{d}^\star)$ over a cross-section defined by $-\frac{t}{2} \leq y \leq \frac{t}{2}$

and $-\frac{h}{2} \leq z \leq \frac{h}{2}$ and integrating the result by part yields

$$\begin{aligned}h^{-1}t^{-1} \int_0^L \int_{-\frac{h}{2}}^{\frac{h}{2}} \int_{-\frac{t}{2}}^{\frac{t}{2}} W(\mathbf{d}^\star) dy dz dx = \\ - \int_0^L \left(2B \frac{d^6 u}{dx^6} + 2(C - A) \frac{d^4 u}{dx^4} + (\lambda + 2\mu) \frac{d^2 u}{dx^2} \right) u^\star(x) dx \\ + \left[u^\star(x) \left(2B \frac{d^5 u}{dx^5} + 2(C - A) \frac{d^3 u}{dx^3} + (\lambda + 2\mu) \frac{du}{dx} \right) \right]_0^L \\ - \left[\frac{du^\star(x)}{dx} \left(2B \frac{d^4 u}{dx^4} + (C - 2A) \frac{d^2 u}{dx^2} \right) \right]_0^L \\ + \left[\frac{d^2 u^\star(x)}{dx^2} \left(2B \frac{d^3 u}{dx^3} + C \frac{du}{dx} + t\tilde{b}_0 \right) \right]_0^L \\ + \int_0^L \left(\frac{Bt^2}{6} \frac{d^8 v}{dx^8} + \left(t^2 \frac{C - A}{6} - 4\tilde{B} \right) \frac{d^6 v}{dx^6} + \left(2\tilde{A} + (\lambda + 2\mu) \frac{t^2}{12} \right) \frac{d^4 v}{dx^4} \right) v^\star(x) dx \\ - \left[v^\star(x) \left(\frac{Bt^2}{6} \frac{d^7 v}{dx^7} + \left(t^2 \frac{C - A}{6} - 4\tilde{B} \right) \frac{d^5 v}{dx^5} + \left(2\tilde{A} + (\lambda + 2\mu) \frac{t^2}{12} \right) \frac{d^3 v}{dx^3} \right) \right]_0^L\end{aligned}$$

$$\begin{aligned}
& + \left[\frac{dv^*(x)}{dx} \left(\frac{Bt^2}{6} \frac{d^6v}{dx^6} + \left(t^2 \frac{C-A}{6} - 4\tilde{B} \right) \frac{d^4v}{dx^4} + \left(2\tilde{A} + (\lambda + 2\mu) \frac{t^2}{12} \right) \frac{d^2v}{dx^2} \right) \right]_0^L \\
& - \left[\frac{d^2v^*(x)}{dx^2} \left(\frac{Bt^2}{6} \frac{d^5v}{dx^5} + \left(t^2 \frac{C-2A}{12} - 4\tilde{B} \right) \frac{d^3v}{dx^3} \right) \right]_0^L \\
& + t \left[\frac{d^3v^*(x)}{dx^3} \left(\frac{Bt}{6} \frac{d^4v}{dx^4} + \frac{Ct}{12} \frac{d^2v}{dx^2} - b_0' \right) \right]_0^L
\end{aligned} \tag{6}$$

where the through-thickness b_0 distribution appears through its projections :

$$\int_{-\frac{t}{2}}^{\frac{t}{2}} b_0(y) dy = t\bar{b}_0 \quad ; \quad \int_{-\frac{t}{2}}^{\frac{t}{2}} b_0(y) y dy = t^2 b_0' \tag{7}$$

The chosen description calls for two remarks :

- Looking at Eq.6 it should be highlighted that the chosen parametrization yields decoupled bending and tension problems. It should however be kept in mind that most of the cantilever sensors applications reported in the literature keep one side of the cantilever unmodified, so that these situations should be described by a change in both \bar{b}_0 and b_0' . As cantilever sensors are commonly based on the detection of the out-of-plane displacement, the tension problem will be discarded in the following.
- The chosen kinematic does not allow for the Poisson effect to develop. As a consequence, the Lamé coefficients appear only

through the combination

$$\lambda + 2\mu = E \frac{1}{1 - \frac{2\nu^2}{1-\nu}} \quad (8)$$

where E and ν stand for the Young's modulus and the Poisson ratio, respectively. In order to approach the Poisson effect without mixing kinematic and static assumptions (as for classical beam theories), it is proposed for the sake of simplicity to replace the combination $\lambda + 2\mu$ by the Young's modulus E everywhere in the following, the identity being obtained for $\nu = 0$ [14]. Mixing kinematic and static assumptions makes here the resulting description useless, especially if one wishes to get closed-form solutions. Any enrichment should therefore be motivated by experimental results.

4 Solutions for the bending problem of a cantilever beam

4.1 General solution

For a cantilever beam clamped at $x = 0$, Eq. 6 (restricted to the tension part) should be satisfied for any test field v^* [15] so that

$$v^*(x) \in \mathcal{V}_{ad} , \mathcal{V}_{ad} = \left\{ v(x) \in H^1([0, L]) \setminus v(0) = 0, \frac{dv}{dx}(0) = 0 \right\} \quad (9)$$

The displacement field should therefore satisfy $\forall x \in [0, L]$

$$\frac{Bt^2}{6} \frac{d^8 v}{dx^8} + \left(t^2 \frac{C - A}{6} - 4\tilde{B} \right) \frac{d^6 v}{dx^6} + \left(2\tilde{A} + E \frac{t^2}{12} \right) \frac{d^4 v}{dx^4} = 0 \quad (10)$$

Looking for solutions of the form

$$v(x) = \exp \left(\Gamma \frac{x}{l_B} \right) \quad (11)$$

Making use of the characteristic lengths defined by Eqs.(1-5) and setting $\tau = \frac{t^2}{6l_B^2}$ the characteristic polynomial in Γ obtained from Eq.(10) reads

$$l_B^2 \tau \Gamma^4 + \left(\tau (l_C^2 - l_A^2) - 4 \frac{l_B^4}{l_B^2} \right) \Gamma^2 + 2l_A^2 + \frac{\tau l_B^2}{2} = 0 \quad (12)$$

The general solution for Eq.(10) therefore reads

$$v(x) = \sum_{i=0}^3 q_i \left(\frac{x}{L} \right)^i + \sum_{j=1}^4 \gamma_j \exp \left(\Gamma_j \frac{x}{l_B} \right) = \sum_{i=0}^3 q_i \left(\frac{x}{L} \right)^i + z(x) \quad (13)$$

where the four Γ_j are the solutions of Eq.(12). The coefficients are to be obtained from the boundary conditions (obtained from both the known displacements and Eq.(6)). The nature (real or complex) of the solutions Γ_j is dictated by the sign of

$$\Delta = \left((l_C^2 - l_A^2)^2 - 2l_B^4 \right) \tau^2 - 8 (l_B^4 l_B^{-2} (l_C^2 - l_A^2) - l_A^2 l_B^2) \tau + \frac{16l_B^8}{l_B^4} \quad (14)$$

and thus depends on the cantilever thickness. It should be highlighted that whatever the material parameters, $\lim_{\tau \rightarrow 0} \Delta = \frac{16l_B^8}{l_B^4} > 0$, so that the zero-thickness limit therefore always corresponds to real solutions for Γ^2 . The discussion of the sign of Δ for a non-vanishing thickness would require the knowledge of the material parameters and is therefore beyond the scope of that paper. One should keep that for a given material, the shape of the general solution may therefore depend on the cantilever's thickness.

4.2 Transverse point-loading

The general solution being defined by Eq.(13), the set of boundary conditions is now solved for a cantilever beam (clamped at $x = 0$) under the action of a transverse point loading F at its tip (no chemical surface change). Adding the corresponding external virtual work to Eq.(6) [15] yields at $x = L$:

$$\begin{aligned} \frac{l_B^4 t^2}{6} \frac{d^7 v}{dx^7} + \left(t^2 \frac{l_C^2 - l_A^2}{6} - 4l_B^4 \right) \frac{d^5 v}{dx^5} + \left(2l_A^2 + \frac{t^2}{12} \right) \frac{d^3 v}{dx^3} &= \frac{F h^{-1} t^{-1}}{E} \quad (15) \\ \frac{l_B^4 t^2}{6} \frac{d^6 v}{dx^6} + \left(t^2 \frac{l_C^2 - l_A^2}{6} - 4l_B^4 \right) \frac{d^4 v}{dx^4} + \left(2l_A^2 + \frac{t^2}{12} \right) \frac{d^2 v}{dx^2} &= 0 \quad (16) \end{aligned}$$

$$\frac{l_B^4 t^2}{6} \frac{d^5 v}{dx^5} + \left(t^2 \frac{l_C^2 - 2l_A^2}{12} - 4l_B^4 \right) \frac{d^3 v}{dx^3} = 0 \quad (17)$$

$$\frac{l_B^4 t}{6} \frac{d^4 v}{dx^4} + t \frac{l_C^2}{12} \frac{d^2 v}{dx^2} = 0 \quad (18)$$

Arranging the Γ_j so that $\Gamma_3 = -\Gamma_1$ and $\Gamma_4 = -\Gamma_2$ and using the facts the Γ_j are solutions for Eq.(12), the system (15-18) is seen to feature six unknowns : q_2, q_3 , as well as the four γ_j . For a cantilever beam, Eq.(6) also yields in $x = 0$

$$\frac{l_B^4 t^2}{6} \frac{d^5 v}{dx^5} + \left(t^2 \frac{l_C^2}{12} - 2l_A^2 - 4l_B^4 \right) \frac{d^3 v}{dx^3} = 0 \quad ; \quad \frac{l_B^4 t}{6} \frac{d^4 v}{dx^4} + t \frac{l_C^2}{12} \frac{d^2 v}{dx^2} = 0 \quad (19)$$

This linear system is solved to yield the displacement field

$$v(x) = q_0 + q_1 \frac{x}{L} + \frac{FL^3}{2htE} \left(2l_A^2 + \frac{t^2}{12} \right)^{-1} \left(- \left(\frac{x}{L} \right)^2 + \frac{1}{3} \left(\frac{x}{L} \right)^3 \right) + z(x) \quad (20)$$

where $z(x)$ is a function vanishing if the lengths defined by Eqs.(1-5) are set to 0. It should be highlighted that l_A^2 is expected to be positive in order to maintain solutions close to the classical solution for any cantilever thickness. The terms q_0 and q_1 are finally set using the clamping conditions :

$$q_0 = - \sum_i \gamma_i \quad ; \quad q_1 = - \sum_i \gamma_i \frac{\Gamma_i}{l_B} \quad (21)$$

It can be easily checked that setting the characteristic lengths to 0 yields the classical solution for an isotropic material. The displacement field depend on all the 6 material parameters, so that these should be identifiable from full-field measurements along tip-loaded cantilever beams of different thicknesses. The defini-

tion of a robust experimental procedure should be investigated. It is however expected the accessible thickness range to drive the identifiability of the involved lengths. This will in turn define some hierarchy among the lengths for a given thickness range.

4.3 Pure chemical loading

Let us now consider a cantilever beam (clamped at $x = 0$) under the action of a heterogeneous chemical surface modification.

Eq.(6) yields at $x = L$:

$$\begin{aligned} \frac{l_B^4 t^2}{6} \frac{d^7 v}{dx^7} + \left(t^2 \frac{l_C^2 - l_A^2}{6} - 4l_B^4 \right) \frac{d^5 v}{dx^5} + \left(2l_A^2 + \frac{t^2}{12} \right) \frac{d^3 v}{dx^3} &= 0 \\ \frac{l_B^4 t^2}{6} \frac{d^6 v}{dx^6} + \left(t^2 \frac{l_C^2 - l_A^2}{6} - 4l_B^4 \right) \frac{d^4 v}{dx^4} + \left(2l_A^2 + \frac{t^2}{12} \right) \frac{d^2 v}{dx^2} &= 0 \\ \frac{l_B^4 t^2}{6} \frac{d^5 v}{dx^5} + \left(t^2 \frac{l_C^2 - 2l_A^2}{12} - 4l_B^4 \right) \frac{d^3 v}{dx^3} &= 0 \\ \frac{l_B^4 t}{6} \frac{d^4 v}{dx^4} + t \frac{l_C^2}{12} \frac{d^2 v}{dx^2} &= \frac{b'_0}{E} \end{aligned}$$

Using the same Γ_j arrangement, and using in $x = 0$

$$\frac{l_B^4 t^2}{6} \frac{d^5 v}{dx^5} + \left(t^2 \frac{l_C^2 - 2l_A^2}{12} - 4l_B^4 \right) \frac{d^3 v}{dx^3} = 0 \quad ; \quad \frac{l_B^4 t}{6} \frac{d^4 v}{dx^4} + t \frac{l_C^2}{12} \frac{d^2 v}{dx^2} = \frac{b'_0}{E} \quad (22)$$

the displacement field reads

$$v(x) = q_0 + q_1 \frac{x}{L} +$$

$$\frac{b'_0 \left(a_1 \sinh \left(\frac{\Gamma_1 L}{2l_B} \right) \cosh \left(\Gamma_2 \frac{2x-L}{2l_B} \right) - a_2 \sinh \left(\frac{\Gamma_2 L}{2l_B} \right) \cosh \left(\Gamma_1 \frac{2x-L}{2l_B} \right) \right)}{tE \left(a_1 b_2 \sinh \left(\frac{\Gamma_1 L}{2l_B} \right) \cosh \left(\frac{\Gamma_2 L}{2l_B} \right) + a_2 b_1 \sinh \left(\frac{\Gamma_2 L}{2l_B} \right) \cosh \left(\frac{\Gamma_1 L}{2l_B} \right) \right)} \quad (23)$$

where q_0 and q_1 result from the clamping condition at $x = 0$ and

where

$$a_i = \frac{l_B^4 t^2}{6} \left(\frac{\Gamma_i}{l_B} \right)^5 + \left(t^2 \frac{l_C^2 - 2l_A^2}{12} - 4l_B^4 \right) \left(\frac{\Gamma_i}{l_B} \right)^3 ; \quad b_i = \frac{l_B^4}{6} \left(\frac{\Gamma_i}{l_B} \right)^4 + \frac{l_C^2}{12} \left(\frac{\Gamma_i}{l_B} \right)^2 \quad (24)$$

. The closed-form solution (23) for the out-of-plane displacement field induced by the chemical modification of one cantilever side calls for several comments :

- It should first be highlighted that this solution, in its generality, may significantly depart from the field resulting from Stoney's assumptions (homogeneous curvature). Besides the rigid-body motion, it may be decomposed into the sum of two hyperbolic cosines with length scales depending on the higher-order elasticity constants. As setting $b_n = c_n = 0$ yields a trivial solution ($q_i = 0$, $\gamma_i = 0$), it is confirmed that a first strain gradient theory is not sufficient to describe surface effects for isotropic materials. This pleads for the use of Mindlin's description, similarly to the elastic fluid described in [17].
- These higher-order elasticity constants necessary reflect the length scales characterizing the material under scrutiny, and

are thus expected to strongly depend on grain size or degree of crystallinity, or more generally, on the processing conditions. The proposed framework therefore seems particularly suited to include the observed dependence on surface morphology [18].

- The role of the cantilever's thickness is much more complicated than it could be envisioned from simple beam theories. Besides the t^{-1} scaling factor, the thickness drives the shape of the displacement field through the solutions of the characteristic polynomial (12), possibly switching the field from hyperbolic to oscillatory (for imaginary solutions). One could easily imagine that such a situation experimentally observed using the (single-point) optical lever technique could lead to some data misinterpretation or ambiguity.
- Besides the thickness, the solution (23) highlights the role of the ratio l_B/L , thus indicating that the cantilever's length could act as a filtering parameter in order to control the amplitude of the component added to the displacement field.

5 Conclusion

An Euler-Bernoulli beam theory for isotropic elastic materials based on a second strain gradient description with a through-

thickness cohesion modulus gradient has been derived. This is thought to accurately describe the mechanical behavior of micro-cantilever sensors, and closed-form solutions are obtained for mechanical and chemical loadings. The proposed modelling involves 6 material parameters which seem to be identifiable from full-field measurements. The shape of the displacement field resulting from a chemical loading is found to possibly significantly depart from the homogeneous curvature assumption resulting from Stoney's assumptions, and depends on the cantilever's thickness as well as on the material parameters. Such a theory may then potentially contribute to explain some of the controversial experimental results found in the literature (when dealing with amorphous or polymeric materials). These potentialities are to be experimentally confirmed and thus require a robust experimental identification procedure of the involved material parameters. The comparison with experimental results should also drive the further developments of such an higher order description.

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